

ABSTRACT

This invention relates to determining the three-dimensional structure of the cytosolic domain of phospholamban (PLB) and its active site from NMR data of sufficiently high resolution for the three-dimensional structure determination. The invention also relates to methods for rational drug design enabling the design of phospholamban inhibitors based on using the three-dimensional structure data provided on computer readable media, as analyzed on a computer system having suitable computer algorithms. The invention also relates to phospholamban inhibiting compounds with certain structural, physicochemical and spatial characteristics that allow for the interaction of said compounds with specific residues of the active site of phospholamban.